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A simple method to obtain very accurate whole atom Compton profiles from photon scattering doubly differential cross sections in relativistic regimes LARRY LAJOHN, University of Pittsburgh — Compton profiles (CP) are used in many ways such as for assessing the bonding properties of molecules and solids including semiconductors. The simplest approach to obtain a CP from doubly differential cross sections (DDCS) is to use the nonrelativistic (nr) impulse approximation (IA) expression DDCS=KJ where K is the kinematic factor and J is the CP. A relativistic version of this expression to be referred to as RKJ, an approximation to the full relativistic IA expression is used for relativistic regimes, but it does not give accurate results for the inner and middle shells of moderate to heavy atoms. For example the RKJ error ranges from 3% (Z=30) to about 28% (Z=92) for the K-shell and about 3% (Z=50) to 17% (Z=92) for the 2p shell and is at 6% for 3d (Z=92). In the present work, expressions from nonrelativistic hydrogenlike wavefunctions (with a relativistic QED K) to correct RKJ beyond the K-shell to L and M shells were derived such that relativistic contributions as well as screening effects largely cancel for any regime of energy angle and Z. As a result the RKJ error is reduced to less than 2% over 99% of the momentum distribution range of any subshell CP.

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